

AD-A033 119

HARRY DIAMOND LABS ADELPHI MD
EXACT EVALUATION OF THE KONDO INTEGRAL.(U)
OCT 76 J L SCALES, N KARAYIANIS, C A MORRISON
HDL-TR-1771

F/G 12/1

UNCLASSIFIED

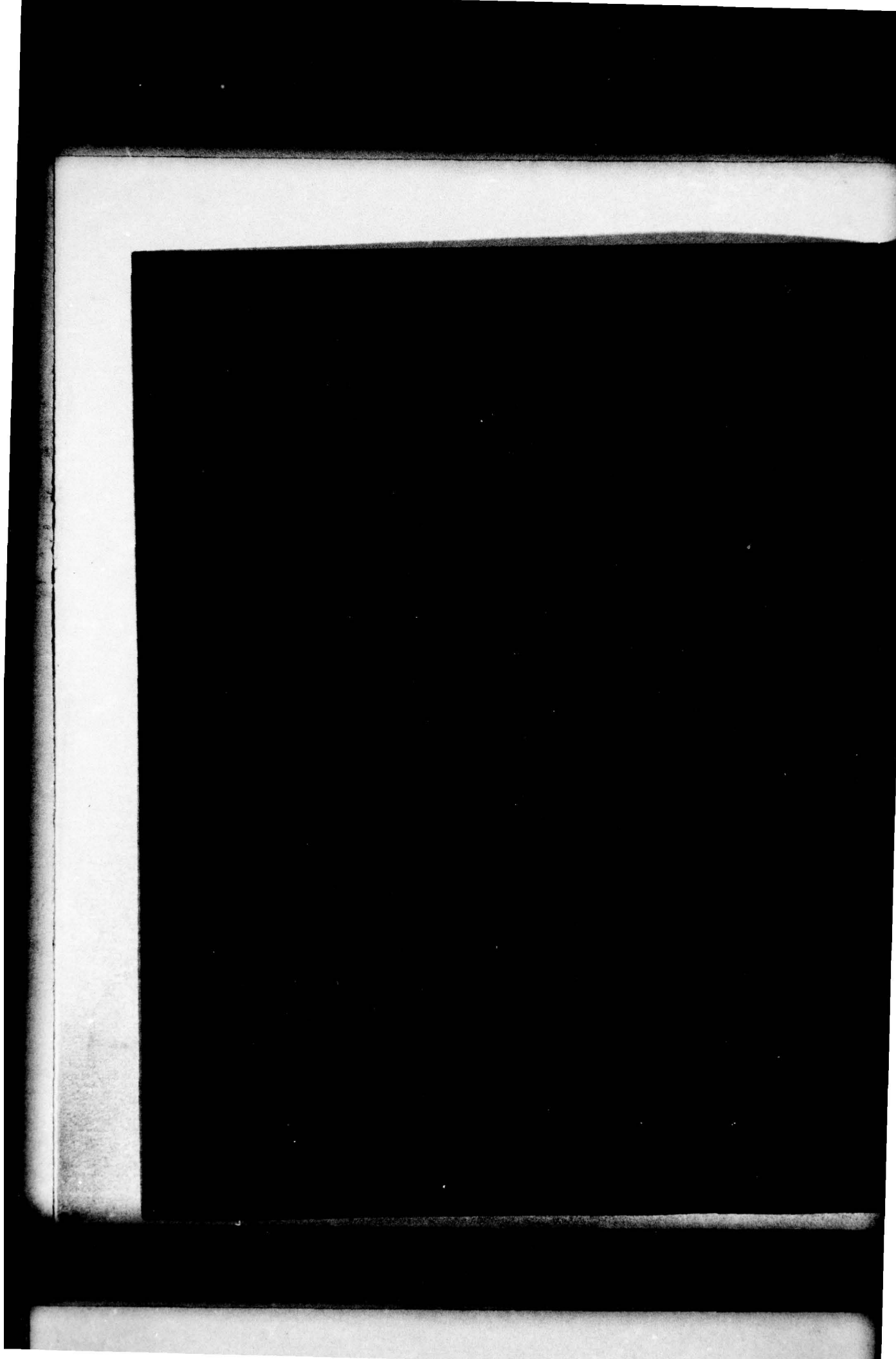
NL

| OF |
AD
A033119



ADA033119

DDC
RECEIVED
DEC 8 1976
RECEIVED



UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER HDL-TR-1771	2. JOINT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Exact Evaluation of the Kondo Integral.	5. TYPE OF REPORT & PERIOD COVERED Technical Report.	
7. AUTHOR(s) John L. Scales Nick Karayianis Clyde A. Morrison	8. CONTRACT OR GRANT NUMBER(s) DA: 1T16102AH46H1	
9. PERFORMING ORGANIZATION NAME AND ADDRESS Harry Diamond Laboratories 2800 Powder Mill Road Adelphi, MD 20783	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS Program: 6.11.02.A	
11. CONTROLLING OFFICE NAME AND ADDRESS U.S. Army Materiel Development & Readiness Command Alexandria, VA 22333	12. REPORT DATE October 1976	
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)	13. NUMBER OF PAGES 24	
15. SECURITY CLASS. (of this report) UNCLASSIFIED	13a. DECLASSIFICATION/DOWNGRADING SCHEDULE	
16. DISTRIBUTION STATEMENT (of this Report) Approved for public release; distribution unlimited.		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report) 16 17161102AH46 12 H1		
18. SUPPLEMENTARY NOTES HDL Project No.: 308637 DRCMS Code: 611102.11.H46H1		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Kondo effect Spin-flip processes		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) A procedure is given for obtaining an exact evaluation of the Kondo integral. This is a mathematical function used to characterize a type of electron scattering; it arises in connection with a variety of physical processes. Previously, there was no exact evaluation of the integral, and various approximation functions were used to represent it. Two of these approximations are compared with the exact answer.		

163050 43

CONTENTS

	<u>Page</u>
1 INTRODUCTION	5
2 FORMULATION	5
3 APPLICATION OF RESULTS	8
4 SUMMARY	11
LITERATURE CITED	12
DISTRIBUTION	23

FIGURES

1. Kondo Function for $E_0 = 10$ meV and $kT = 0.1$ meV	9
2. Kondo Function for $E_0 = 2$ meV and $T = 1.25$ K	10

TABLE

I Numerical Values for the Function $H(y) = \ln(2\pi) - 1$ $+ \operatorname{Re} \Psi(1+iy/2\pi) + yd/dy \operatorname{Re} \Psi(1+iy/2\pi)$	8
---	---

APPENDICES

A.--CONTOUR INTEGRAL NO. 1	13
B.--CONTOUR INTEGRAL NO. 2	17
C.--CORRECTION TERM FOR FINITE CUTOFF	21

ACCESSION for	
NTIS	White Section <input checked="" type="checkbox"/>
DIC	Bull Section <input type="checkbox"/>
UNANNOUNCED	<input type="checkbox"/>
JUSTIFICATION	
BY	
DISTRIBUTION/AVAILABILITY CODES	
Dist.	A.A.U. RND/OF SPECIAL
A	



1. INTRODUCTION

A dilute alloy composed of a magnetic impurity dissolved in a nonmagnetic host may exhibit anomalous resistivity at low temperature. Kondo¹ explained the phenomenon by taking into account the spin-spin interaction between conduction electrons and immobile ions. He showed that this led--in third-order perturbation theory--to a resistivity having logarithmic dependence on temperature. The same type of electron-ion coupling has been used to explain other phenomena. For example, Kondo scattering has been invoked to explain anomalous tunneling in thin-film structures² and Schottky-barrier junctions,³ and to explain negative magnetoresistance in semiconductor materials.⁴

Until now, no exact evaluation of the Kondo integral has been reported. Applebaum⁵ performed a numerical integration and suggested an approximation function to represent his results. Wolf and Losee⁶ also did a numerical evaluation, but they suggested a different approximation function. The work reported here gives an exact evaluation of the integral in terms of analytic functions.

2. FORMULATION

Let the Kondo integral be defined as

$$F(y,c) = - \int_{-\infty}^{\infty} g(x,c) \frac{d}{dx} f(x-y) dx \quad (1)$$

where $f(x)$ is the Fermi function. The function $g(x,c)$ is defined as

$$g(x,c) = \mathcal{P} \int_{-c}^c \frac{f(t) - \frac{1}{2}}{t - x} dt \quad (2)$$

where \mathcal{P} denotes principal value of the integral, and c is a cutoff parameter. Equation (2) can be integrated by parts. Proper care must

¹J. Kondo, *Prog. Theoret. Phys. (Kyoto)* **32** (1964), 37.

²J. Appelbaum, *Phys. Rev. Lett.* **17** (1966), 91.

³P. W. Anderson, *Phys. Rev. Lett.* **17** (1966), 95.

⁴R. P. Khosla and J. R. Fischer, *Phys. Rev.* **2B** (1970), 4084.

⁵J. Appelbaum, *Phys. Rev.* **154** (1967), 633.

⁶E. L. Wolf and D. L. Losee, *Phys. Rev.* **B2** (1970), 3660.

be taken with the singularity at $t = x$, and it is noted that $\ln|t - x|$ is the integral of $(t - x)^{-1} dt$ for both $t > x$ and $t < x$. Therefore, the result is

$$g(x, c) = -[f(-c) - \frac{1}{2}] \ln|c + x| + [f(c) - \frac{1}{2}] \ln|c - x| - \int_{-c}^c f'(t) \ln|t - x| dt. \quad (3)$$

The next step is to substitute equation (3) into equation (1) and perform the integration. For this it is useful to have the result proved in appendix A, namely

$$J(a) = -\int_{-\infty}^{\infty} f'(t) \ln|t - a| dt = \ln(2\pi) + \operatorname{Re} \Psi(\frac{1}{2} + ia/2\pi). \quad (4)$$

In equation (4) Re denotes the real part of the complex function, and Ψ is the digamma function.⁷ Using equation (4), one can substitute equation (3) into equation (1) and obtain the following:

$$\begin{aligned} F(y, c) = & -[f(-c) - \frac{1}{2}] \{ \ln 2\pi + \operatorname{Re} \Psi[\frac{1}{2} - i(c + y)/2\pi] \} \\ & + [f(c) - \frac{1}{2}] \{ \ln 2\pi + \operatorname{Re} \Psi[\frac{1}{2} + i(c - y)/2\pi] \} \\ & - \int_{-c}^c f'(t) \{ \ln 2\pi + \operatorname{Re} \Psi[\frac{1}{2} - i(t + y)/2\pi] \} dt. \end{aligned} \quad (5)$$

In the problems of physical interest, such as tunneling and anomalous resistivity in alloys, the parameter c has a magnitude of the order of 100. In such cases, it is an excellent approximation to let $f(-c) \rightarrow 1$, $f(c) \rightarrow 0$, and use the large-argument approximation for the digamma function, i.e.,

$$\operatorname{Re} \Psi[\frac{1}{2} \pm ix] \approx \ln x. \quad (6)$$

With these approximations, equation (5) reduces to the form

$$F(y, c) = -\frac{1}{2} \ln|c^2 - x^2| - \int_{-c}^c f'(t) \operatorname{Re} \Psi[\frac{1}{2} - i(t + y)/2\pi] dt. \quad (7)$$

⁷M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions*, U.S. Government Printing Office, Washington, D.C. (1964), 258.

Appendices B and C show how to perform the integration in equation (7). For $c \rightarrow \infty$, the integration can be performed by using the theory of residues (shown in appendix B). Then a correction term is derived for finite c (shown in appendix C). For any problem of physical interest, the correction term is very small because the major contributions to the integral in equation (7) come from those regions near $t = 0$ and $t = -y$. The integrand decreases rapidly for large t , and, if c is large, the integral has almost the same value for finite c as for $c \rightarrow \infty$. Using the results developed in appendices B and C, one can write the exact evaluation of the Kondo integral as

$$F(y,c) = -\frac{1}{2}\ln|c^2 - y^2| + \ln(2\pi) - 1 + \operatorname{Re} \Psi(1 + iy/2\pi) + y \frac{d}{dy} \operatorname{Re} \Psi(1 + iy/2\pi) + K(y,c) . \quad (8)$$

As before, Re denotes the real part of the complex variable, and Ψ is the digamma function. The term $K(y,c)$ in equation (8) is the correction term for finite c that was developed in appendix C.

A discussion of the Kondo function follows in section 3 of this report. First, however, a remark may be made concerning the function $g(x,c)$ given in equation (3). Certainly the principal dependence of g on c is embodied in the first two terms of equation (3); little error is incurred by letting the limits on the integral become infinite. Therefore one can use equation (4) to write

$$g(x,c) = -\ln(c^2 - x^2) + \ln(2\pi) + \operatorname{Re} \Psi(\frac{1}{2} + ix/2\pi) . \quad (9)$$

This agrees with the result given by Bloomfield and Hamann,⁸ (their equation A-8), but they "derived" the digamma function by deducing a recurrence relation, and then arguing that the recurrence relation defined the function to within an additive constant. Actually, the recurrence relation of the digamma function defines it only to within an additive function, since, for example, $\psi(z) + A \sin(\pi z)$ obeys the same recurrence relation as $\psi(z)$.

⁸P. Bloomfield and D. R. Hamann, *Phys. Rev.* 164 (1967), 856.

3. APPLICATION OF RESULTS

Table I gives numerical values of the function

$$H(x) = \ln(2\pi) - 1 + \operatorname{Re} \Psi\left(\frac{1}{2} + ix/2\pi\right) + x \frac{d}{dx} \operatorname{Re} \Psi\left(\frac{1}{2} + ix/2\pi\right). \quad (10)$$

TABLE I. NUMERICAL VALUES FOR THE FUNCTION
 $H(y) = \ln(2\pi) - 1 + \operatorname{Re} \Psi(1 + iy/2\pi) + y \frac{d}{dy} \operatorname{Re} \Psi(1 + iy/2\pi)$

y	Re Ψ	d/dy (Re Ψ)	H(y)
0.0	-0.5772	0.0000	0.2607
0.1	-0.5769	0.0382	0.2616
0.2	-0.5760	0.0764	0.2643
0.3	-0.5745	0.1143	0.2689
0.4	-0.5724	0.1520	0.2752
0.5	-0.5696	0.1892	0.2833
0.6	-0.5663	0.2260	0.2931
0.7	-0.5625	0.2622	0.3046
0.8	-0.5580	0.2977	0.3178
0.9	-0.5530	0.3325	0.3325
1.0	-0.5474	0.3665	0.3488
1.1	-0.5413	0.3996	0.3665
1.2	-0.5347	0.4317	0.3856
1.3	-0.5276	0.4628	0.4061
1.4	-0.5200	0.4929	0.4277
1.5	-0.5119	0.5219	0.4506
1.6	-0.5034	0.5497	0.4745
1.7	-0.4944	0.5763	0.4994
1.8	-0.4850	0.6017	0.5252
1.9	-0.4753	0.6259	0.5519
2.0	-0.4651	0.6489	0.5793
2.1	-0.4546	0.6706	0.6074
2.2	-0.4438	0.6911	0.6361
2.3	-0.4326	0.7103	0.6653
2.4	-0.4212	0.7283	0.6949
2.5	-0.4094	0.7451	0.7249
2.6	-0.3975	0.7606	0.7552
2.7	-0.3852	0.7750	0.7857
2.8	-0.3728	0.7882	0.8163
2.9	-0.3602	0.8003	0.8471
3.0	-0.3473	0.8113	0.8779
3.1	-0.3343	0.8212	0.9087
3.2	-0.3212	0.8301	0.9394
3.3	-0.3079	0.8380	0.9701
3.4	-0.2945	0.8449	1.0006
3.5	-0.2810	0.8509	1.0308
3.6	-0.2674	0.8560	1.0609
3.7	-0.2538	0.8603	1.0907
3.8	-0.2401	0.8638	1.1202
3.9	-0.2263	0.8665	1.1494
4.0	-0.2125	0.8685	1.1783

This is the Kondo function without the terms that depend on the parameter c . Values in table I were calculated from a series representation of the digamma function,⁸ i.e.,

$$\operatorname{Re} \Psi\left(\frac{1}{2} + iy\right) = -\gamma + \sum_{n=1}^{\infty} \frac{y^2}{n(n^2 + y^2)} . \quad (11)$$

The summations were continued until the last term was less than 10^{-7} times the sum of the preceding terms; the same rule was used for calculating the derivative of equation (11).

Figure 1 compares the correct Kondo function and the approximation used by Appelbaum.⁵ His approximation function was

$$F \text{ approx} = -\ln[(y + 1)/c] . \quad (12)$$

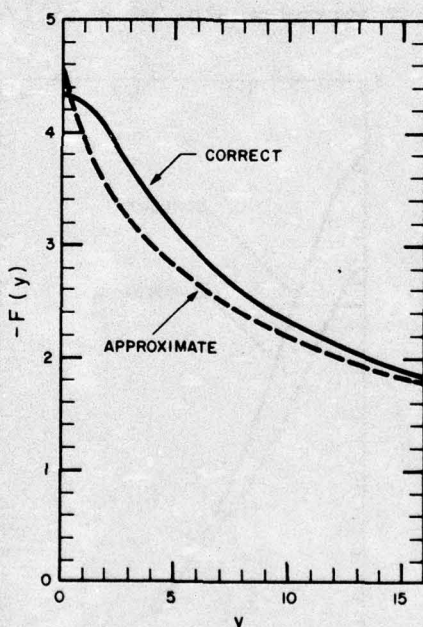


Figure 1. Kondo function for $E_0 = 10$ meV and $kT = 0.1$ meV, corresponding to $c = E_0/kT = 100$. The dashed curve is the approximation used by Appelbaum.

⁵J. Appelbaum, *Phys. Rev.* **154** (1967), 633.

⁸P. Bloomfield and D. R. Hamann, *Phys. Rev.* **164** (1967), 856.

This function has finite slope at $y = 0$, whereas the correct Kondo function has zero slope. The value of the parameter used in figure 1 was $c = 100$, corresponding to Appelbaum's cutoff energy $E_0 = 10$ meV at a temperature $kT = 0.1$ meV; thus $c = E_0/kT = 100$. The Kondo function has smaller slope than the approximation function, especially as $y \rightarrow 0$. This difference could be important. For example, in the theory of magnetoresistance, y is the ratio of magnetic energy, μB , to thermal energy, kT . For a magnetic moment of one Bohr magneton, in a field of one kilogauss, at the temperature of liquid helium, $y = \mu B/2\pi kT = 10^{-3}$. This is small and, furthermore, one uses the derivative of the Kondo function to analyze magnetoresistance data. Misleading results would be obtained if one used the approximation function instead of the correct function in this case.

Figure 2 compares the correct Kondo function with the approximation function used by Wolf and Losee.⁶ Their approximation function was

$$F \text{ approx} = -\ln[(y^2 + \alpha^2)^{1/2}/c] . \quad (13)$$

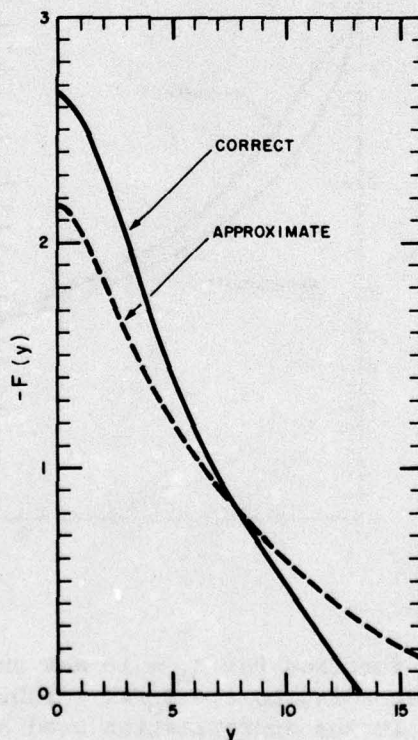


Figure 2. Kondo function for $E_0 = \frac{1}{2}$ meV and $T = 1.25$ K, corresponding to $c = E_0/kT = 18.55$. The dashed curve is the approximation function of Wolf and Losee with $\alpha = 2.12$.

⁶E. L. Wolf and D. L. Losee, *Phys. Rev. B2* (1970), 3660.

This function has the correct slope at $y = 0$, but the wrong magnitude at $y = 0$ unless α is chosen properly. Wolf and Losee used the value $\alpha = 2.12$, which causes $F(y)$ to be too large at $y = 0$. Also, the correct Kondo function has larger slope than the approximation function for all $y > 0$.

Shen and Rowell³ stated that the result of a numerical integration of the integral

$$\ln \beta = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f'(t) f'(x) \ln |t - x| dx dt \quad (14)$$

was $\beta \approx 1.35$. The exact result, obtained from appendix B, is

$$\ln \beta = \ln(2\pi) - 1 - \gamma. \quad (15)$$

This gives the correct value, $\beta = 1.2978$.

Problems of physical interest frequently require an evaluation of the Kondo function at values of the argument small compared with unity. In such cases, it is convenient to use an approximation of the digamma function derived from equation (11), i.e.,

$$\operatorname{Re} \Psi(\frac{1}{2} + iy) = -\gamma + y^2 \zeta(3), \quad (16)$$

where $\zeta(3) = 1.202$ is the zeta polynomial. Then the Kondo function can be written

$$f(y, c) = -\ln c + a + by^2 \quad (17)$$

where $a = \ln(2\pi) - 1 - \gamma = 0.2607$, and $b = 3\zeta(3)/(2\pi)^2 = 0.0776$.

4. SUMMARY

The Kondo function, defined in equations (1) and (2), was evaluated by contour integration and shown to be expressible in the form given in equation (8). This differs slightly from the approximation functions used by various authors. For example, the correct function has zero slope at the origin, whereas the function suggested by Appelbaum had finite slope. The function used by Wolf and Losee had correct slope at the origin, but the magnitude was incorrect. In general, the correct function has larger slope than the Wolf and Losee function and smaller slope than the Appelbaum function, for $y > 0$. A definite integral mentioned by Shen and Rowell was evaluated exactly and found to have a smaller value than the approximate value they quoted.

³L. Y. L. Shen and J. M. Rowell, *Phys. Rev.* 165 (1968), 566.

LITERATURE CITED

- (1) J. Kondo, Prog. Theoret. Phys. (Kyoto) 32 (1964), 37.
- (2) J. Appelbaum, Phys. Rev. Lett. 17 (1966), 91.
- (3) P. W. Anderson, Phys. Rev. Lett. 17 (1966), 95.
- (4) R. P. Khosla and J. R. Fischer, Phys. Rev. 2B (1970), 4084.
- (5) J. Appelbaum, Phys. Rev. 154 (1967), 633.
- (6) E. L. Wolf and D. L. Losee, Phys. Rev. B2 (1970), 3660.
- (7) M. Abramowitz and I. Stegun, Handbook of Mathematical Functions, U.S. Government Printing Office, Washington, D.C. (1964), 258.
- (8) P. Bloomfield and D. R. Hamann, Phys. Rev. 164 (1967), 856.
- (9) L. Y. L. Schen and J. M. Rowell, Phys. Rev. 165 (1968), 566.

APPENDIX A.--CONTOUR INTEGRAL NO. 1

Consider the contour integral

$$I(a) = - \oint f'(z) \ln(z - a) dz , \quad (A-1)$$

where the path is defined in figure A-1 and

$$f'(z) = -1/[4 \cosh^2(z/2)] . \quad (A-2)$$

A branch cut is taken along the real axis from $u = -\infty$ to $u = a$; thus the logarithm is understood to be

$$\ln(z - a) = \ln|z - a| + i\phi \quad (A-3)$$

where ϕ is the angle shown in figure A-1.

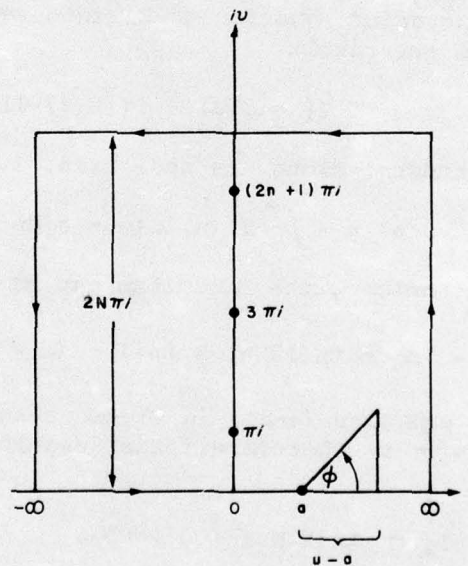


Figure A-1. Contour in the complex plane used in evaluating the integral of equation (A-1).

APPENDIX A

The function $f'(z)$ has second-order poles at $z = i\pi(2n + 1)$, where $n = 0, 1, 2, \dots$, and the residue of the integrand at the n^{th} pole is

$$R_n = [a - i\pi(2n + 1)]^{-1}. \quad (\text{A-4})$$

The contours encloses N poles, and the procedure is to take the limit as $N \rightarrow \infty$, after the integral has been evaluated for finite N .

The integration consists of four parts: integration along the real axis, I_1 , integration along the top contour parallel to the real axis, I_2 , and integration along the two vertical legs. The latter contribute nothing because $f'(z) \rightarrow 0$ as the real part of $z \rightarrow \pm\infty$. Therefore, according to the theory of residues, the result can be written as

$$I_1 + I_2 = 2\pi i \sum_{n=0}^{N-1} R_n. \quad (\text{A-5})$$

Along the real axis, the phase angle is $\phi = \pi$ for $u < a$, and $\phi = 0$ for $u > a$. Substitution of equation (A-3) into equation (A-1) therefore leads immediately to the result

$$I_1 = J(a) - i\pi[f(a) - 1], \quad (\text{A-6})$$

where $J(a)$ is the integral along the real axis, i.e.

$$J(a) = - \int_{-\infty}^{\infty} f'(u) \ln|u - a| du. \quad (\text{A-7})$$

Along the upper contour, the logarithm can be written

$$\ln(u + i2N\pi - a) = \ln(i2N\pi) + \ln[1 + (u - a)/i2N\pi]. \quad (\text{A-8})$$

The second term in equation (A-8) is less than $(u - a)/i2N\pi$, which approaches zero as $N \rightarrow \infty$. Therefore, the result of integration along the upper path is

$$I_2 = -\ln(i2N\pi) + O(1/N). \quad (\text{A-9})$$

Using these results, one has

$$J(a) - i\pi[f(a) - 1] - \ln(2iN\pi) = 2\pi i \sum_{n=0}^N [a - i\pi(2n + 1)]. \quad (\text{A-10})$$

APPENDIX A

Let $\xi = \frac{1}{2} + i(a/2\pi)$. Then the term on the right side of equation (A-10) can be written as

$$\sum_{n=0}^{N-1} \frac{2\pi i}{a - i\pi - (2n + 1)} = \frac{1}{\xi} + \sum_{n=1}^{N-1} \left[\frac{\xi}{n(n + \xi)} \right] - \frac{1}{n}. \quad (\text{A-11})$$

A series representation of the digamma function¹ is

$$\Psi(1 + \xi) = -\gamma + \sum_{n=0}^N \frac{\xi}{n(n + \xi)}, \quad (\text{A-12})$$

where γ is the Euler constant defined as

$$\gamma = \lim_{N \rightarrow \infty} \left[\sum_{n=1}^N \left(\frac{1}{n} \right) - \ln N \right]. \quad (\text{A-13})$$

Using the recurrence relation

$$\Psi(1 + \xi) = \Psi(\xi) + 1/\xi, \quad (\text{A-14})$$

one can write equation (A-11) as

$$J(\xi) = i\pi[f(a) - \frac{1}{2}] + \ln 2\pi + \Psi(\xi). \quad (\text{A-15})$$

Note that the imaginary part of $\Psi(\frac{1}{2} + iy)$ is $(\pi/2) \tanh \pi y$, which means that $\text{Im} \psi(\xi)$ exactly cancels the first term in equation (A-15). The final result is

$$J(a) = \ln 2\pi + \text{Re } \psi[\frac{1}{2} + (ia/2\pi)]. \quad (\text{A-16})$$

¹M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions*, U.S. Government Printing Office, Washington, D.C. (1964), 259.

APPENDIX B.--CONTOUR INTEGRAL NO. 2

The object is to show that $H(x)$ defined as

$$H(x) = - \int_{-\infty}^{\infty} f'(t) \operatorname{Re} \Psi[\frac{1}{2} + i(t+x)/2\pi] dt \quad (B-1)$$

can be expressed as

$$H(x) = -1 + \operatorname{Re} \psi(1 + ix/2\pi) + x \frac{d}{dx} [\operatorname{Re} \psi(1 + ix/2\pi)] . \quad (B-2)$$

An integral representation of the digamma function is¹

$$\Psi(s) = -\gamma + \int_0^{\infty} \frac{\exp(-u) - \exp(-su)}{1 - \exp(-u)} du . \quad (B-3)$$

The procedure is to substitute equation (B-3) into equation (B-1), letting $s = \frac{1}{2} + i(t+x)/2\pi$. One can perform two trivial integrations immediately. Then, having interchanged the order of integration in the third term, one obtains

$$H(x) = -\gamma + \int_0^{\infty} \frac{\exp(-u) du}{1 - \exp(-u)} - \operatorname{Re} \int_0^{\infty} \frac{\exp[-u(\frac{1}{2} + ix/2\pi)]}{1 - \exp(-u)} \int_{-\infty}^{\infty} f'(t) \exp(-i t/2\pi) dt dw . \quad (B-4)$$

The t -integral in equation (B-4) can be done by contour integration. Consider the function

$$I(a) = \int \frac{\exp[z(1 - ia)] dz}{[1 + \exp(z)]^2} \quad (B-5)$$

defined by the contour shown in figure B-1. The denominator of equation (B-5) has second-order poles at $z = \pi i(2n + 1)$, $n = 0, 1, 2, \dots$, and the contour encloses one of these poles. The residue at $z = \pi i$ is $R = i a \exp(\pi a)$. Let the integral along the real axis be I_1 , and the integral along the upper leg, parallel to the real axis, be I_2 . I_2 is the same as I_1 , except that the variable in I_2 is $z = u + 2\pi i$, instead of $z = u$, as it is in I_1 . This introduces only a multiplicative factor, so that

$$I_2(a) = -\exp(2\pi a) I_1(a) . \quad (B-6)$$

¹M. Abramowitz and I. Stegun, Handbook of Mathematical Functions, U.S. Government Printing Office, Washington, D.C. (1964), 259.



APPENDIX B

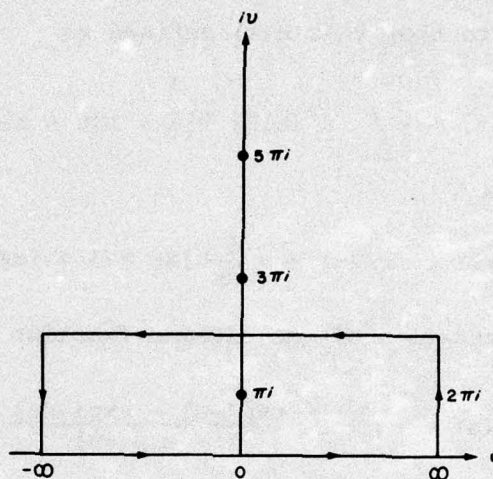


Figure B-1. Contour in the complex plane used in evaluating the integral of equation (B-1).

The integrals along the vertical legs do not contribute anything because the integrand in equation (B-5) approaches zero as $u \rightarrow \pm\infty$. Therefore, according to residue theory, the result of the contour integration is

$$I_1 [1 - \exp(2\pi a)] = +2\pi a \exp(\pi a), \quad (B-7)$$

which becomes

$$I_1(a) = \frac{\pi a}{\sinh(\pi a)}. \quad (B-8)$$

Except for a minus sign, the t -integral in equation (B-4) is the same as $I_1(a)$, with $a = x/2\pi$. Therefore, equation (B-8) can be substituted into equation (B-4), and the result written as

$$H(x) = -\gamma + \int_0^\infty \frac{\exp(-u) du}{1 - \exp(-u)} + \operatorname{Re} \int_0^\infty \frac{u \exp[-u(1 + ix/2\pi)] du}{[1 - \exp(-u)]^2} \quad (B-9)$$

APPENDIX B

The last term in equation (B-9) can be integrated by parts. The procedure is to use

$$\int_0^{\infty} f dg = f g \Big|_0^{\infty} - \int_0^{\infty} g df \quad (B-10)$$

where

$$f(u) = u \exp(1 - ux/2\pi) , \quad (B-11)$$

and

$$g(u) = -\exp(-u)/[1 - \exp(-u)] . \quad (B-12)$$

This leads to the result

$$H(x) = -\gamma + \int \frac{\exp(-u) du}{1 - \exp(-u)} - 1 - \operatorname{Re} \int_0^{\infty} \frac{(1 - iux/2\pi) \exp[-u(1 + ix/2\pi)] du}{1 - \exp(-u)} . \quad (B-13)$$

By using (B-3), one can rewrite this as

$$H(x) = -1 + \operatorname{Re} \psi(1 + ix/2\pi) + x \frac{d}{dx} [\operatorname{Re} \psi(1 + ix/2\pi)] . \quad (B-14)$$

This is the result claimed.

APPENDIX C.--CORRECTION TERM FOR FINITE CUTOFF

This appendix will show that the error incurred by letting $c \rightarrow \infty$ in equation (5) of the body of this report is acceptably small. The amount added to the integral when the upper limit approaches infinity is

$$K(x,c) = - \int_c^{\infty} f'(t) \operatorname{Re} \Psi[\frac{1}{2} + i(t+x)/2\pi] dt . \quad (C-1)$$

The duplication formula¹ for the digamma function gives

$$\Psi(\frac{1}{2} + iy) = 2\Psi(2iy) - \Psi(iy) - 2\ln 2 . \quad (C-2)$$

An asymptotic expansion of the digamma function is

$$\operatorname{Re} \Psi(iy) = \ln y + (12y^2)^{-1} + (120y^4)^{-1} + \dots \quad (C-3)$$

From equations (C-1) and (C-2), one can obtain the result

$$\operatorname{Re} \Psi(\frac{1}{2} + iy) = \ln y - (24y^2)^{-1} - 7(960y^4)^{-1} - \dots \quad (C-4)$$

Since $-f'(t) > \exp(-t)$ for $t \ll 0$, it is permissible to rewrite equation (C-1) as the following inequality:

$$K(x,c) < \int_c^{\infty} \exp(-t) \ln[(t+x)/2\pi] dt . \quad (C-5)$$

Integration by parts gives

$$K(x,c) < \exp(-c) \ln[(C+x)/2\pi] + \int_c^{\infty} \exp(-t) (t+x)^{-1} dt . \quad (C-6)$$

The integral is less than $\exp(-c)$. Therefore, the final result can be written as

$$K(x,c) < \exp(-c) \{1 \pm \ln[(t+x)/2\pi]\} . \quad (C-7)$$

Sample values of the correction term are $K(5,10) > 4.6 \times 10^{-5}$, and $K(10,10) < 5.3 \times 10^{-9}$. These are small compared with the values of the corresponding integrals.

¹N. Abramowitz and I. Stegun, Handbook of Mathematical Functions, Dover Publications, Inc. (1965), 259.

DISTRIBUTION

DEFENSE DOCUMENTATION CENTER
CAMERON STATION, BUILDING 5
ALEXANDRIA, VA 22314
ATTN DDC-TCA (12 COPIES)

COMMANDER
USA RSCH & STD GP (EUR)
BOX 65
FPO NEW YORK 09510
ATTN LTC JAMES M. KENNEDY, JR.
CHIEF, PHYSICS & MATH BRANCH

COMMANDER
US ARMY MATERIEL DEVELOPMENT
& READINESS COMMAND
5001 EISENHOWER AVENUE
ALEXANDRIA, VA 22333
ATTN DRXAM-TL, HQ TECH LIBRARY

COMMANDER
USA ARMAMENT COMMAND
ROCK ISLAND, IL 61201
ATTN DRSAR-ASF, FUZE DIV
ATTN DRSAR-RDF, SYS DEV DIV - FUZES

COMMANDER
USA MISSILE & MUNITIONS
CENTER & SCHOOL
REDSTONE ARSENAL, AL 35809
ATTN ATSK-CTD-F

CHEMISTRY/METALLURGY DIVISION
AMES LABORATORY
US ENERGY RES & DEV ADMIN
IOWA STATE UNIVERSITY
AMES, IA 50012

US DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS
WASHINGTON, DC 20230

DIRECTOR OF DEFENSE RESEARCH
& ENGINEERING
WASHINGTON, DC 20301
ATTN ASST DIR (ELECTRONICS
& PHYSICAL SCIENCES)

ASSISTANT SECRETARY OF THE ARMY (R&D)
WASHINGTON, DC 20310
ATTN DEP FOR SCI & TECH

OFFICE, CHIEF OF RESEARCH,
DEVELOPMENT & ACQUISITION
DEPARTMENT OF THE ARMY
WASHINGTON, DC 20310
ATTN DAMA-AR, RESEARCH PROGRAMS

COMMANDER
US ARMY ELECTRONICS COMMAND
FT. MONMOUTH, NJ 07703
ATTN DRSEL-RD, DIR, RESEARCH, DEV, & ENGR

COMMANDER
US ARMY MATERIALS & MECHANICS RESEARCH
CENTER
WATERTOWN, MA 02172
ATTN TECHNICAL LIBRARY

COMMANDER
FRANKFORD ARSENAL
BRIDGE & TACONY STREETS
PHILADELPHIA, PA 19137
ATTN L1000, PITMAN-DUNN LABORATORY
CHIEF OF RES DIV
ATTN L5000, APPLIED SCI DIV

CHIEF OF NAVAL RESEARCH
DEPT OF THE NAVY
ARLINGTON, VA 22217
ATTN ONR-421, ELECT & SOLID STATE
SCI PROG

DIRECTOR
NAVAL RESEARCH LABORATORY
WASHINGTON, DC 20375
ATTN CODE 2620, LIBRARY
ATTN CODE 4000, RESEARCH DEPT

SUPERINTENDENT
AIR FORCE ACADEMY
COLORADO SPRINGS, CO 80840
ATTN TECH LIB

COMMANDER
AEROSPACE RESEARCH LABORATORIES
WRIGHT-PATTERSON AFB, OH 45433
ATTN LS, SOLID STATE PHYSICS RES LAB

COMMANDER
AF CAMBRIDGE RESEARCH LABORATORIES, AFSC
L. G. HANSCOM FIELD
BEDFORD, MA 01730
ATTN LQ, SOLID-STATE SCI LAB

DIRECTOR
AF OFFICE OF SCIENTIFIC RESEARCH
1400 WILSON BLVD
ARLINGTON, VA 22209
ATTN NM, DIR OF MATHEMATICAL & INFO SCI

AMES RESEARCH CENTER
NASA
MOFFETT FIELD, CA 94035
ATTN DIR OF RESEARCH SUPPORT



DISTRIBUTION (Cont'd)

DIRECTOR

NASA

GODDARD SPACE FLIGHT CENTER

GREENBELT, MD 20771

ATTN 250, TECH INFO DIV

DIRECTOR

NASA

JOHN F. KENNEDY SPACE CENTER, FL 32899

ATTN TECHNICAL LIBRARY

HARRY DIAMOND LABORATORIES

ATTN MCGREGOR, THOMAS, COL, COMMANDING

OFFICER/FLYER, I.N./LANDIS, P.E./

SOMMER, H./CONRAD, E.E.

ATTN CARTER, W.W., DR., ACTING TECHNICAL

DIRECTOR/MARCUS, S.M.

ATTN KIMMEL, S., IO

ATTN CHIEF, 0021

ATTN CHIEF, 0022

ATTN CHIEF, LAB 100

ATTN CHIEF, LAB 200

ATTN CHIEF, LAB 300

ATTN CHIEF, LAB 400

ATTN CHIEF, LAB 500

ATTN CHIEF, LAB 600

ATTN CHIEF, DIV 700

ATTN CHIEF, DIV 800

ATTN CHIEF, LAB 900

ATTN CHIEF, LAB 1000

ATTN RECORD COPY, BR 041

ATTN HDL LIBRARY (3 COPIES)

ATTN CHAIRMAN, EDITORIAL COMMITTEE

ATTN CHIEF, 047

ATTN TECH REPORTS, 013

ATTN PATENT LAW BRANCH, 071

ATTN MCLAUGHLIN, P.W., 741

ATTN LANHAM, C., PROGRAM & PLANS

ATTN SCALES, J., 540 (5 COPIES)

ATTN KARAYIANIS, N., 320 (5 COPIES)

ATTN MORRISON, C., 320 (5 COPIES)

ATTN CAMPI, M., 240

ATTN GIBSON, H., 540